

ABSTRACT OF THE DISCLOSURE

The present invention relates to crystals of the *Escherichia coli* MurG, a membraneassociated UDP-glycosyltransferase involved in peptidoglycan biosynthesis. The present invention also 5 relates to three-dimensional atomic coordinates of the MurG protein, three-dimensional structures of the protein, and images thereof. The present invention also relates to the atomic coordinates and three-dimensional structures of the α -carbon backbone and of the α -carbon backbone and conserved amino acid residue sidechains of the MurG protein and images thereof. The present invention further relates to three-dimensional atomic coordinates of the donor nucleotide binding 10 site, the acceptor binding site, and the membrane association site of the MurG protein, three-dimensional structures of the binding domains, and images thereof. The present invention also relates to computer readable media encoded with sets of the three dimensional coordinates described herein. The present invention relates to methods of crystallizing MurG proteins. The present invention relates to models of three dimensional structures of UDP-glycosyltransferases and, in particular, MurG proteins, based on the three dimensional structure of crystals of the *Escherichia coli* MurG. The present invention also relates to models of the three dimensional structures of the α -carbon backbone and the α -carbon backbone and conserved amino acid residue sidechains of UDPglycosyltransferases and MurG proteins and of the binding sites thereof, The present invention also relates to methods of drug design using models of this invention, the compounds identified using models of the present invention that bind, inhibit or stimulate UDP-glycosyltransferases or MurG proteins, and compositions comprising compounds identified using the models of this invention for therapeutic or diagnostic uses. Also, the present invention relates to methods of making models of the present invention.

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